Soft X-ray Emission and Absorption Spectra of Base Molecules, Deoxy-Ribose, and DNA in the C *K*, N *K*, and O *K* Regions

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Electronic structure analysis of biological molecules has been required to understand their physicochemical reactions in radiation chemistry/biology. For example, Akamatsu [1] recently reported the physicochemical changes of 2-deoxy-D-ribose molecules under the monochromatized x-ray irradiation. We therefore measured the soft x-ray emission and absorption spectra of essential biological molecules (base molecules, deoxy-ribose, and DNA), and compared these x-ray spectra with calculated spectra to analyze their electronic structures. Powder samples of adenine (denoted by A), guanine (G), cytosine (C), thymine (T), 2-deoxy-D-ribose (dR), and DNA were commercially obtained, and their soft x-ray emission and absorption spectra in C *K*, N *K*, and O *K* regions were measured in BL-8.0.1 and BL-6.3.2. Calculated spectra were obtained by discrete-variational (DV) -Xα molecular orbital calculation method. Figure 1 shows the x-ray emission spectra of the base molecules, deoxy-ribose, and DNA, and their calculated density of state (DOS) spectra of occupied C2p, N2p, and O2p orbitals. Spectral feature differences in the x-ray emission spectra were observed among the samples, and the calculated DOS spectra approximately agree with the x-ray spectral features. Further theoretical analysis of the x-ray emission and absorption spectra is in progress to determine the electronic structure of the biological molecules.

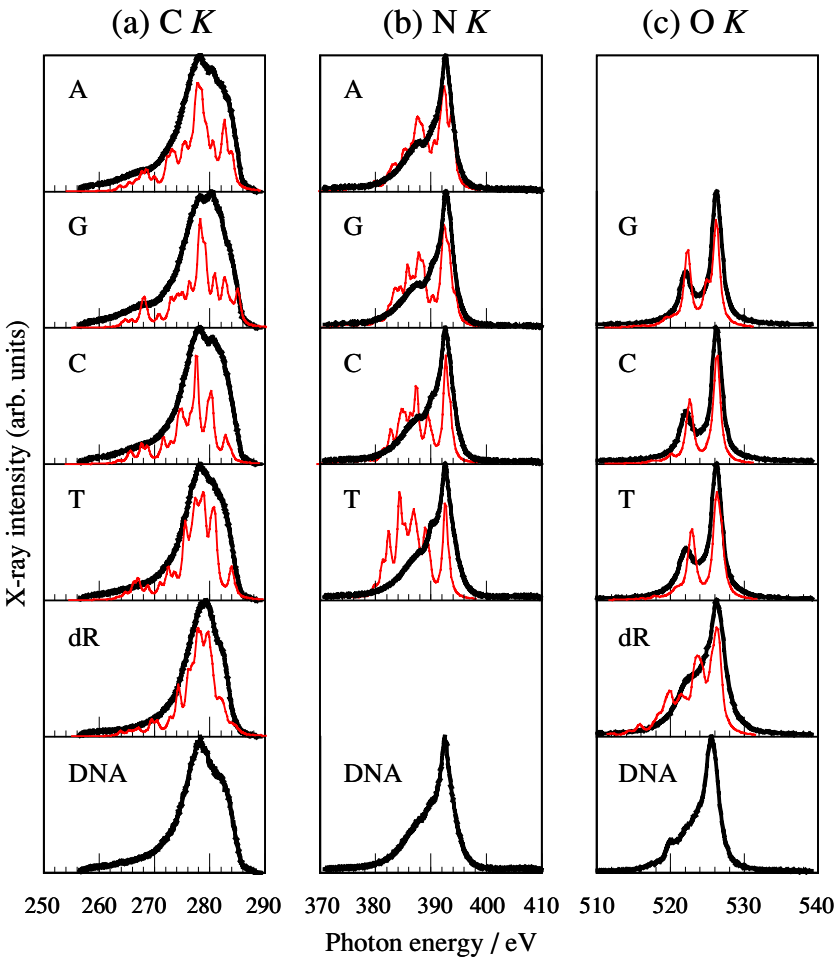

Figure 1. Soft x-ray emission spectra (bold lines) of base molecules (A, G, C, T), deoxy-ribose (dR), and DNA in the (a) C *K*, (b) N *K*, and (c) O *K* regions. Occupied C2p-, N2p-, and O2p-DOS spectra of base molecules and deoxy-ribose are superimposed on the corresponding x-ray emission spectra.

[1] K. Akamatsu et al., J. Synchrotron Radiation (in press).

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